

# Multiscale simulation of the nanometric cutting process

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## Abstract

Molecular dynamics (MD) simulation and finite element (FE) method are two popular numerical techniques for the simulation of machining processes. The two methods have their own strengths and limitations. The MD simulation can cover the phenomena occurring at nanometric scale lengths but limited by the computational cost and capacity, while FE method is suitable for modelling the meso to macro scale machining and for simulating macro parameters such as the temperature in a cutting zone, the stress/strain distribution and cutting forces, etc. With the successful application of multiscale simulations in many research fields, the application to simulate machining processes is emerging particularly in relation to the machined surface generation and integrity formation, i.e. the machined surface roughness, residual stress, microhardness, microstructure and fatigue.

Based on the Quasicontinuum (QC) method, the multiscale simulation of nanometric cutting has been proposed. Cutting simulations are performed on single crystal aluminium to investigate the chip formation, generation and propagation of the material dislocation during the cutting process. In addition, the effect of the tool rake angle on cutting force and internal stress under the workpiece surface is investigated. The cutting force and internal stress in the workpiece material decrease with the increase of the rake angle. Finally, to ease and speed up multiscale modelling and simulation steps, a computing efficient MATLAB-based program has been developed, which facilitates the geometrical cutting modelling, simulation conditions, implementation of simulation and results analysis within a unified integrated virtual simulation environment.

**Keywords:** Multiscale simulation, Molecular dynamics, Finite element method, Nanometric cutting

## Nomenclature

$E_i$	energy contribution from site $x_i$
$E_{tot}$	total energy
$N_e$	the number of elements.
$N_{rep}$	the number of representative atoms involved
$S_\alpha$	finite element shape function

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$u_j$  displacement of non-representative atoms

$\alpha$  representative atoms

$\varepsilon(A)$  strain energy density

$x_j^0$  the initial position of atom  $j$

$\Omega_k$  unit cell volume

$n_\alpha$  a suitably chosen weight

$A$  deformation gradient

$E_\alpha$  energy of each repatom

$u_\alpha$  displacement of each repatom

MD molecular dynamic

QC quasi continuum

EAM embedded atom method

## 1. Introduction

The nanometric cutting is very complex because of the size effect, elastic/plastic deformation and fracture with high strain rates, and varying material properties during the cutting process. Analytical modelling is thus considered extremely difficult at the current level of understanding of the material behaviour. Most analytical modelling efforts are based on kinematics from empirical observation combined with classic cutting models at the macro level. The applicability and accuracy of these models are subject to many limitations [1].

Although involving many assumptions as the analytical model does, the numerical modelling and simulation of nanometric cutting provides a powerful tool for assisting scientific understanding of the cutting physics, chip formation mechanisms, size-effects, and the machined surface integrity. Using the numerical model and simulation, the effect of various cutting conditions can be emulated and manipulated easily and effectively while it also leads to reducing costly physical cutting trials and the process optimisation. Finite element (FE) modelling and molecular dynamics (MD) modelling are two popular numerical modelling and simulation techniques for the investigation of machining processes although each technique has its own strengths and limitations.

FE method is based on the principle of continuum mechanics, in which the materials are defined as continuous structure and effects of micro-constituents such as crystal structure, grain size, and inter-atomic distances are ignored. Application of FE simulation to the cutting process provides an effective means to understand the mechanics and characteristics of the cutting process. It has been used successfully for the prediction of cutting forces, temperature distribution and stress distribution, etc, with a practical accuracy at the macro level [2-5]. However, FE method can not be used for the simulation of nanometric cutting because the constitutive equations have vital errors when the mesh size approaches to the atomic scale. At nanoscale, the expression for the elastic energy does not represent localized bonds and the standard distributed mass expression for

the kinetic energy does not account for the fact that essentially all of the mass is localized in the atomic nuclei, i.e. at least four orders of magnitude smaller than the interatomic spacing [6]. Therefore, FE method is not suitable for the simulation of nanometric cutting due to the inappropriate physics of governing equations.

Molecular dynamics (MD) simulation is a well established methodology for detailed microscopic modelling at a molecular scale. It is based upon the molecules model of the matter or system concerned according to their atomic structures. Potential functions are used to describe the molecular interactions, and the interatomic forces can be derived from the differentiation of the potential function. In this case, MD simulation is suitable for nanometric cutting. It can specially perform the study of the tool-workpiece interaction [7], the effect of crystallographic orientation and direction on cutting which is very difficult to obtain in FE simulation [8, 9]. On the other hand, MD simulation has limitations on examining large structures and computational speed and time, the number of atoms considered in the workpiece material is thus rather small in most published MD cutting simulation. Such limitations may cause some unwanted computational artificial results from small model boundaries. To bring the MD simulation closer to realistic nanometric cutting conditions, the size of the simulation must be increased dramatically beyond that which has been presently reported [6]. Therefore, the multiscale modelling is much needed so as to reduce the computational cost and enlarge the simulation scale, efficiency and effectiveness while maintaining the simulation resolution.

A natural approach to the multiscale simulation is to combine MD and FE method, in which MD is used for the modelling of the critical regions within the system while FE is applied for the continuum description of the remainder of the system. The hybrid approach provides an atomistic description at the interface and a continuum description deep into substrate, increasing the accessible length scales and greatly reducing the computational cost. There have been a number of applications where the FE method is used to simulate an adequate static and dynamic response of surrounding material to the process in the MD computational cell [10-14]. The emerging multiscale modelling will likely play an important role in the characterization of the machining process at reduced size scales, particularly in explaining phenomenological effects across the nano-micro-meso continuum [15]. To date, however, few multiscale simulation has been applied to the machining process [6, 16], although it shows considerable promise for dealing with the multiplicity of issues that arise over multiple scales in the machining process. Several multiscale simulation methods have been developed such as the FEAt method, the Quasicontinuum (QC) method, the MAAD method, and the CGMD method, although they are merely applied in other domains.

In this paper, multiscale simulations based on QC method are presented to examine the chip formation, generation, propagation of atomic dislocations and other cutting physics aspects during the nanometric cutting process to investigate the effect of the rake angle on the cutting force and internal stress. Furthermore, the development of a MATLAB-based simulation system is presented, which provides the users with a high interactive user-friendly QC modelling and simulation environment.

## 2. QC method

QC method originally proposed by Tadmor et al. in 1996 [17] is an outstanding multiscale simulation approach. The idea underlying this method is that atomistic calculation resolution is required only in regions with high gradients, but the description of regions with slowly varying gradients follows well-established continuum finite element theories. Thus, the degrees of freedom and computational requirement are reduced significantly without losing atomistic detail in interested regions. Furthermore, the fully atomistic, critical regions can evolve with the deformation during the simulation [18]. Generally, the QC method consists of the following three main components:

- (1) A FE method on an adaptively generated mesh, which is automatically refined to the atomistic level near defects;
- (2) A kinematic constraint by which representative atoms are selected;
- (3) The Cauchy-Born rule that computes an approximation to the total energy of the system by visiting only a small subset of the atoms.

Ideally, in order to calculate the total energy, one needs to visit all the atoms in the domain:

$$E_{tot} = \sum_{i=1}^N E_i(x_1, x_2, \dots, x_N) \quad (1)$$

Here  $E_i$  is the energy contribution from site  $x_i$ . The precise form of  $E_i$  depends on the potential function used. In the region where the displacement field is smooth, keeping track of each individual atom is unnecessary. Therefore, some representative atoms (repatoms) can be selected to reduce the computational cost. After selecting repatoms, the displacement of any atoms in the system is obtained from a finite element mesh which is constructed with repatoms as nodes. The approximate displacement of non-representative atoms can be obtained by interpolation:

$$u_j = \sum_{\alpha=1}^{N_{rep}} S_{\alpha}(x_j^0) u_{\alpha}$$

where the subscript  $\alpha$  identifies the representative atoms.  $S_{\alpha}$  is an finite element shape function.

$N_{rep}$  is the number of repatoms involved.

Though this step reduces the number of degrees of freedom to be calculated, it still need to visit every atom. To reduce the computational complexity involved in obtaining the total energy, several simplified rules are introduced. One of these rules, namely that the Cauchy-Born rule assumes that the deformation gradient,  $A$ , is uniform within each element. The strain energy in the element  $\Omega_k$  can be approximately written as  $\varepsilon(A_k)|\Omega_k|$  in terms of the strain energy density  $\varepsilon(A)$ . With these approximations, the evaluation of the total energy is reduced to a summation over the finite elements:

$$E_{tot} \approx \sum_{k=1}^{N_e} \varepsilon(A_k) |\Omega_k| \quad (2)$$

where  $N_e$  is the number of elements. This formulation is called the local version of QC.

In the presence of material defects, the deformation tends to be non-smooth. Therefore, the approximation made in local QC will be inaccurate. A non-local version of QC has been developed in which the energy is expressed as:

$$E_{tot} \approx \sum_{\alpha=1}^{N_{rep}} n_{\alpha} E_{\alpha}(u_{\alpha}) \quad (3)$$

Here  $n_{\alpha}$  is a suitably chosen weight. The energy from each repatom  $E_{\alpha}$  is computed by visiting its neighboring atoms whose positions are generated by the local deformation. Practical implementation usually combines both local and non-local version of the method, and a criterion has been proposed to identify the local/non-local regions, so that the whole procedure can be applied adaptively.

QC has been successfully applied to a number of problems including dislocation structure, nanoindentation, crack propagation, and deformation twinning.

### 3. Multiscale modelling and simulation

#### 3.1 Modelling and simulation on nanometric cutting of single crystal aluminium

Fig.1 shows the multiscale simulation model applied to the nanometric cutting of single crystal aluminium. To investigate the workpiece material behaviour, formation of chip, generation of machined surface during cutting process, atomistic calculation resolution is performed along the workpiece surface, while the region away from the interested tool-workpiece interaction is estimated based on the finite element theory. So it can be seen from the multiscale model of cutting that the atom density becomes larger upwards, and the material is represented exactly with atoms at the material upper surface. The size of the work material is  $0.2 \times 0.1 \mu\text{m}$ , and the number of material atoms in the initial model is 10, 263. At the 50th step time the number of material atoms is no more than 20, 000, which is much less compared to  $1.25 \times 10^7$  atoms included in its MD model. The computational intensity is greatly reduced by using the quasicontinuum method.

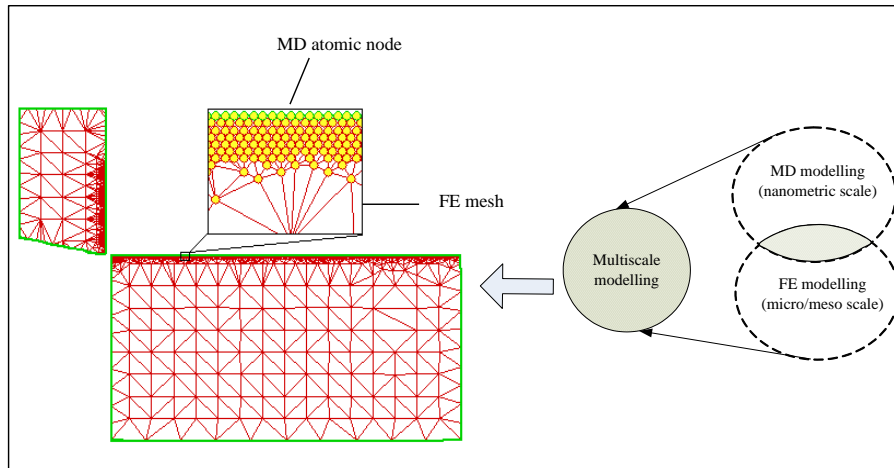


Fig.1 Multiscale model for nanometric cutting of single crystal Aluminum

The simulation is conducted on the single crystal aluminium along the crystal orientation  $\langle 001 \rangle$  and cutting direction  $[100]$  with the depth of cut 1 nm. For convenience, an infinitely hard diamond tool is used in the simulation because tool wear is hardly a problem at machining pure aluminium. The constitutive law for aluminium is chosen as the embedded atom method (EAM) potential for the simulation. The nanometric cutting is performed by gradually moving the tool relative to the workpiece with each step of 0.3 angstrom. Table 1 lists the computational parameters used in the simulation.

Table 1 Parameters used in the multiscale simulation of the nanometric cutting of single crystal aluminium

Configuration	2D
Workpiece material	Single crystal aluminium
Potential function	EAM
Workpiece dimensions	$0.2 \times 0.1 \mu\text{m}$
The number of work atoms (initial value)	10263
Tool rake angle	$0^\circ$
Tool clearance angle	$10^\circ$
Depth of cut	1nm

The advantages of combining the MD and FE methods together in the context of multiscale modelling and simulation of the cutting process are:

- (1) The modelling and simulation can cover a large surface area machined with comprehensive surface integrity information including surface roughness, microhardness, microstructure changes at subsurface, residual stress and fatigue, etc.
- (2) The application of FE method for the continuum description of the non-critical area within the system is able to eliminate the atomistic degrees of freedom and thus improve the computation efficiency.
- (3) The combination of MD and FE can preserve atomistic details, such as atom dislocation, in the surface generation area and continuum information, such as residual stress, at the workpiece subsurface.

## 3.2 Results and discussions

### 3.2.1 The process of nanometric cutting

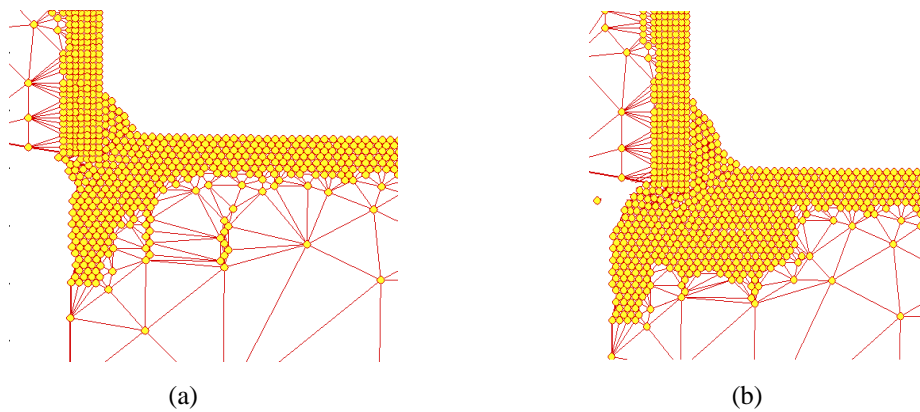


Fig. 2 The atom snapshot with motion of the tool: (a) at the 20<sup>th</sup> time step; (b) at the 43<sup>rd</sup> time step

Although the QC method can describe larger volumes with fewer atoms, its efficiency depends on the performance of computer hardware because it is not a high-speed algorithm. In the multiscale simulation, we only obtained 43 time step results due to condition limitations. Fig.2 shows the atom snapshot at the 20<sup>th</sup> time step and the 43<sup>rd</sup> time step of the cutting process simulation.

At the start, the uncut material in the workpiece seems to be little affected by the motion of the tool because little meshes beneath the tool are refined to atomic level (Fig.2 (a)). As the cutting progresses, not only the material ahead of the tool is deformed, but several layers below the uncut material ahead of the tool tip is also affected (Fig.2 (b)) since meshes of the deformed material are refined to the atomic level.

Under the effect of the cutting tool, the workpiece atoms are piled up along the front face of the cutting tool as the atom cluster (Fig.2 (a)), and with the progress of the cutting they are removed in the form of chips (Fig.2 (b)). As the tool passes the machined surface, partial elastic recovery of the deformed subsurface region takes place and the remained deformation results in the subsurface deformation beneath the machined surface (Fig.2 (b)). It can be seen obviously that the generation and propagation of dislocations into the workpiece material at an angle of 0°~45°. All phenomena mentioned above are very similar to the results obtained by the MD simulation [8], which means the application of multiscale QC to nanometric cutting is feasible.

### 3.2.2 The effect of rake angle on cutting force and internal stress

Fig.3 shows the cutting forces obtained with two different rake angles, 0° and 30°. It can be seen that cutting force decreases when the rake angle increases. The mean cutting force during the machining process is 1.65 nN with a rake angle of 0°, and it is reduced to 0.54 nN when the rake angle is set at 30°. These multiscale simulation results of nanometric cutting force are very close to the MD simulation results produced by Luo [19].

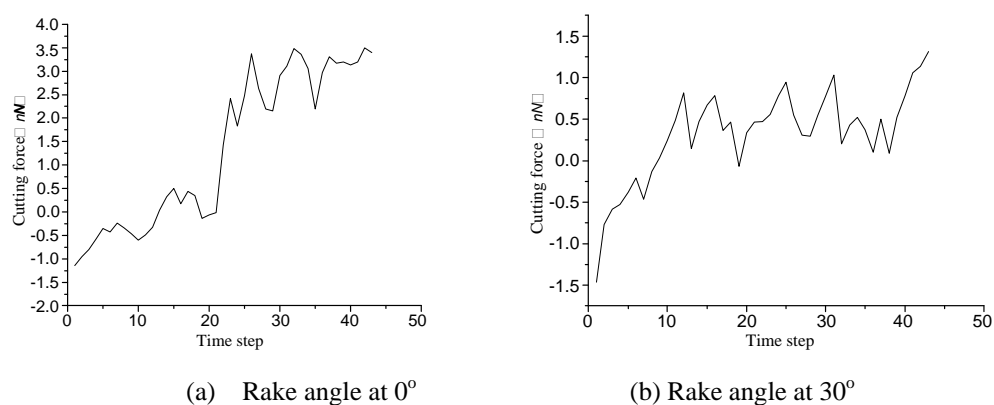


Fig.3 The variation of cutting force during machining process

The internal stress in the workpiece at the 43<sup>rd</sup> time step is depicted in Fig.4 for different rake angles. The maximum stress in the workpiece is 2.4 MPa and 1.5 MPa when the rake angle is 0° and 30°, respectively. The results indicate that smaller rake angle results in greater internal stress.

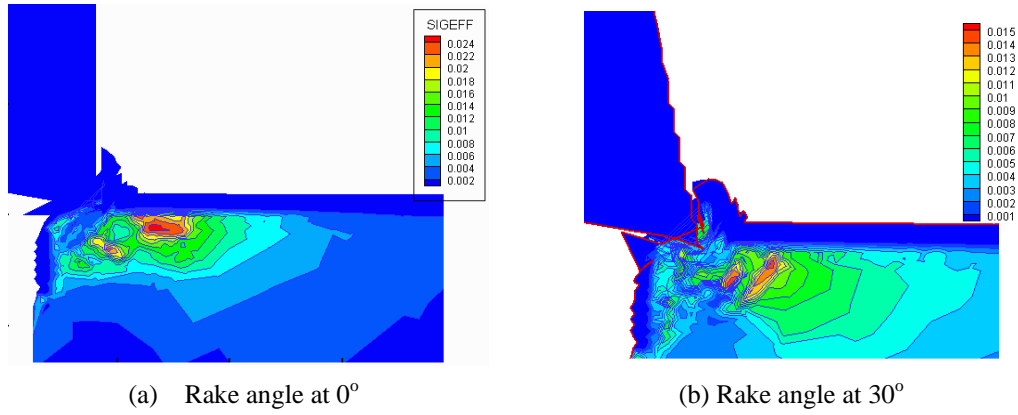


Fig.4 The stress contour in the workpiece at 43<sup>rd</sup> time step

#### 4. Modelling and simulation environment and its implementation

Whilst the application of QC method to nanometric cutting is successful, the procedure of the simulation and results analysis are more complex. For example, parameters such as material properties, potential function, model parameters, cut-off radius, step time and other simulation parameter in parameter inputs file have to be defined separately by the user. The geometrical model in the simulation is also expressed in the text format, which is not intuitive to users. To provide users with a user-friendly and highly productive integrated environment for the QC simulation of nanometric cutting, a MATLAB-based simulation system has been developed.

The system provides tool and workpiece geometrical parameters description, simulation conditions, implementation of QC, simulation results analysis within a unified visual environment and can execute on Windows operation system. This system has significantly simplified and speeded up the modelling and simulation steps. The integration of modelling, simulation and analysis can enable the QC simulations of nanometric cutting to behave a virtual nanometric cutting system.

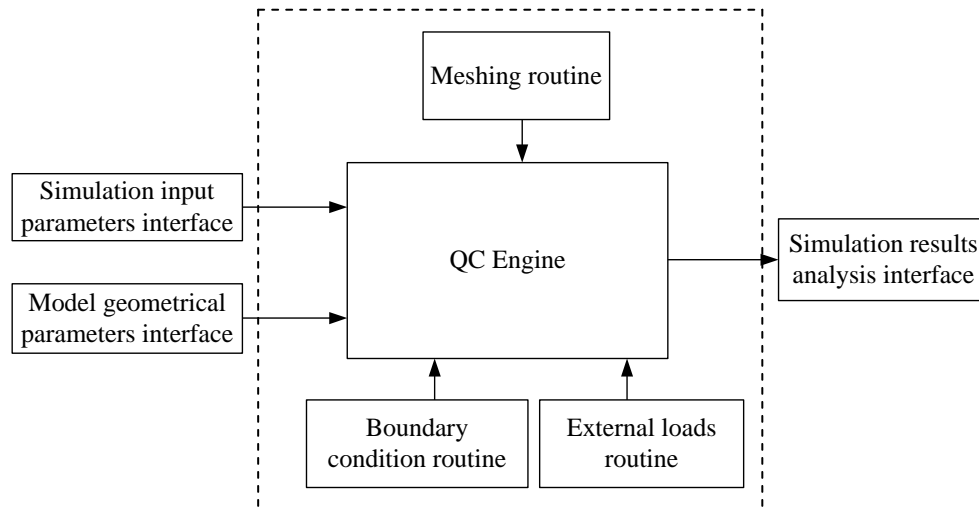


Fig.5. Architecture of the simulation system

The architecture of the simulation system is illustrated in Fig.5. The meshing routine, boundary condition routine and external loads routine are compiled by the QC engine with an executable file generated in advance. Given the data defined through the simulation parameters input interface



and the model geometrical parameters interface, the executable file can perform the required cutting simulation. Simulation results can be obtained from simulation results analysis interface.



Fig.6 The main interface of the simulation system

The screen copy of the system main interface illustrated in Fig.6 provides the interactive selection access for different functions of the system, each with a prompt message. The functions buttons are listed in the typical order of the simulation process, but each of them can be chosen and run independently. If necessary, default parameters can be used in the simulation.

In the Model Geometrical Parameters interface (Fig.7), the standard cutting configuration is shown with both the tooling and the workpiece. A number of geometrical parameters have been defined with default values displayed, such as the size of the workpiece, the shape of the tool, etc. Through the interface, the user can edit and change the values of these parameters according to the needs of each particular application. When the OK button is clicked, all the changes made will be saved and subsequently used in the simulation. If EXIT is clicked, the changes will be discarded and the default values will be used instead in the simulation.

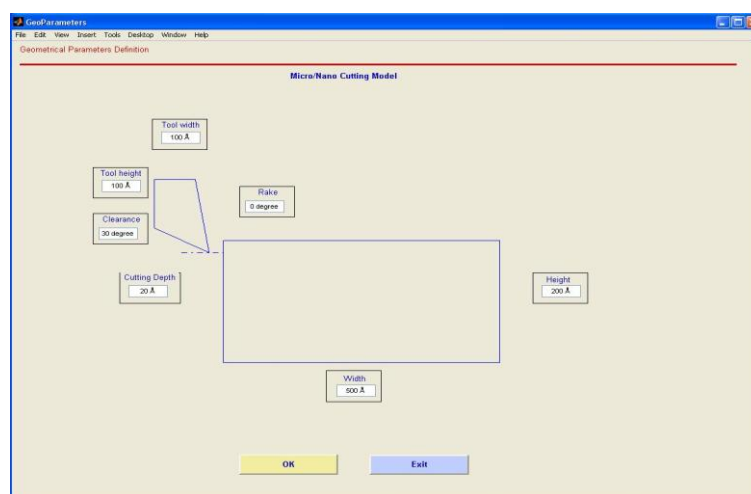


Fig.7 Geometrical Parameters input interface

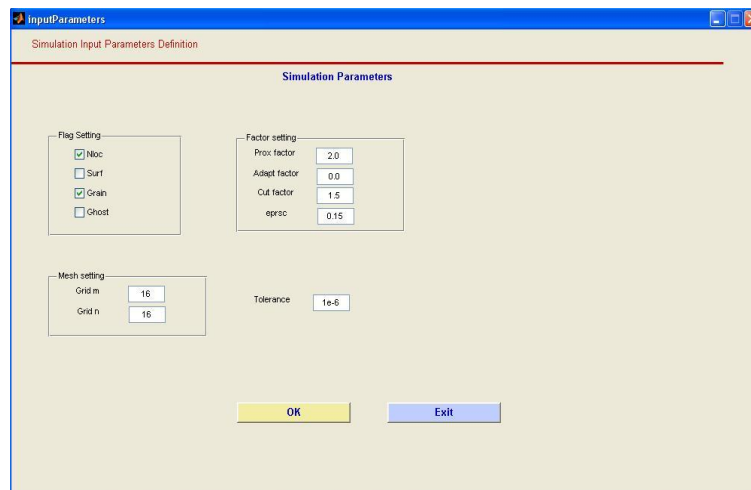


Fig.8 Simulation Input Parameters interface

The Simulation Input Parameters interface (shown in Fig. 8) has several groups of controls, i.e. a group of check boxes for simulation flag settings, a group of text boxes for simulation factor settings, a pair of text boxes for mesh setting and a text box for simulation tolerance setting. Again, each of the settings has a default value, but the user can freely change the settings according to the requirements. The changes can also be saved or discarded by clicking the OK or EXIT button.

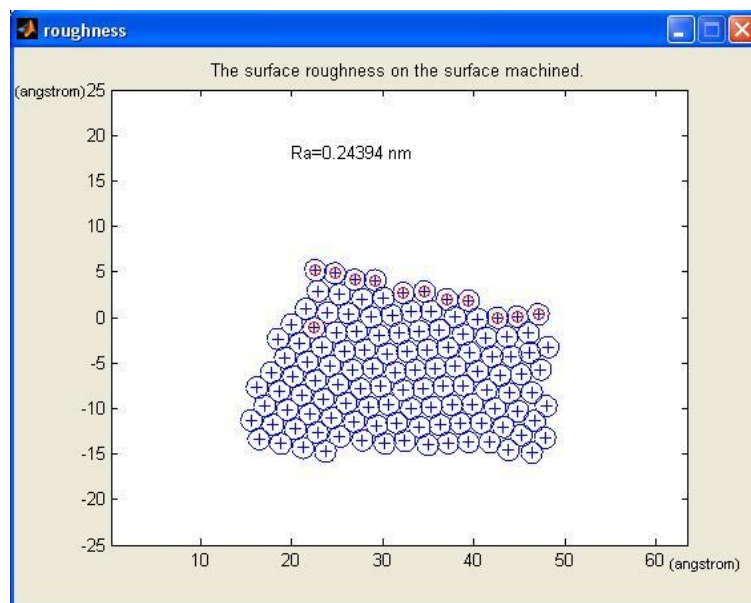


Fig. 9 The roughness of the machined surface

One example of the simulation results analysis is shown in Fig.9, in which the roughness of the machined surface is calculated. The results are generated in four steps: 1) The results analysis module firstly displays the initial distributions of the atoms of both the tooling and workpiece. 2) The atoms of machined surface are displayed. 3) The user defines the beginning and the finishing atoms of the surface to be evaluated. 4) The program then calculates the Ra value according to its definition based upon the distribution of the atoms concerned. More analysis functions can be similarly performed, e.g. cutting force in the cutting process and residual stress at the machined surface.

## 5. Cutting trials: evaluation and validation

### 5.1 Experimental design

The above modelling and simulation results have been evaluated and validated with some basic experimental results, and a generally good agreement has been achieved. In order to validate the models against more practical applications, the following experiments and cutting trials have been designed, based upon the response surface method (Box-Behnken design), as shown in Table 2. Four key factors have been chosen in the experiments, i.e. tool nose radius (0.1 – 3 mm), tool rake angle ( $-5^\circ$  –  $0^\circ$ ), depth of cut (0.1 – 5  $\mu\text{m}$ ) and cutting speed (50 – 150 m/min). The experiments will study the surface roughness and residual stress as the main responses.

Table 2 Box-Behnken experiment layout

Exp. No.	Tool nose radius (mm)	Tool rake angle	Depth of cut( $\mu\text{m}$ )	Cutting speed (m/min)	Tool nose radius (mm)	Tool rake angle	Depth of cut( $\mu\text{m}$ )	Cutting speed (m/min)
1	1	1	2	2	0.1	$0^\circ$	3	100
2	1	3	2	2	0.1	$-5^\circ$	3	100
3	3	1	2	2	3	$0^\circ$	3	100
4	3	3	2	2	3	$-5^\circ$	3	100
5	2	2	1	1	0.5	$-2.5^\circ$	0.1	50
6	2	2	1	3	0.5	$-2.5^\circ$	0.1	150
7	2	2	3	1	0.5	$-2.5^\circ$	5	50
8	2	2	3	3	0.5	$-2.5^\circ$	5	150
9	1	2	2	1	0.1	$-2.5^\circ$	3	50
10	1	2	2	3	0.1	$-2.5^\circ$	3	150
11	3	2	2	1	3	$-2.5^\circ$	3	50
12	3	2	2	3	3	$-2.5^\circ$	3	150
13	2	1	1	2	0.5	$0^\circ$	0.1	100
14	2	1	3	2	0.5	$0^\circ$	5	100
15	2	3	1	2	0.5	$-5^\circ$	0.1	100
16	2	3	3	2	0.5	$-5^\circ$	5	100
17	1	2	1	2	0.1	$-2.5^\circ$	0.1	100
18	1	2	3	2	0.1	$-2.5^\circ$	5	100
19	3	2	1	2	3	$-2.5^\circ$	0.1	100
20	3	2	3	2	3	$-2.5^\circ$	5	100
21	2	1	2	1	0.5	$0^\circ$	3	50
22	2	1	2	3	0.5	$0^\circ$	3	150
23	2	3	2	1	0.5	$-5^\circ$	3	50
24	2	3	2	3	0.5	$-5^\circ$	3	150
25	2	2	2	2	0.5	$-2.5^\circ$	3	100
26	2	2	2	2	0.5	$-2.5^\circ$	3	100
27	2	2	2	2	0.5	$-2.5^\circ$	3	100

## 5.2 Experiment setup

The experimental setup is shown in Fig. 10. A 3-axis diamond turning machine tool developed at Brunel University will be used for the experimental trials. The different geometrical diamond cutting tools used are provided by Contour Fine Tooling Ltd. The air bearing spindle on the 3-axis diamond turning machine has the maximum rotational speed of 15,000 rpm.

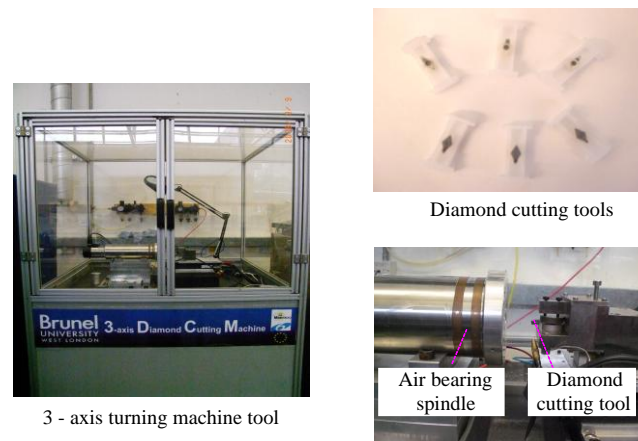


Fig. 10 The experiment setup

## 5.3 Evaluation and validation

The procedure for further evaluation and validation of the QC model is proposed as depicted in Fig. 11. The simulations and cutting trials are performed under the same cutting conditions according to the above experimental design in the same order as defined by the Box-Behnken design. Once the trials are completed, the simulation and experimental results can then be directly compared. If necessary, the models can be continuously refined until satisfactory agreement to be achieved.

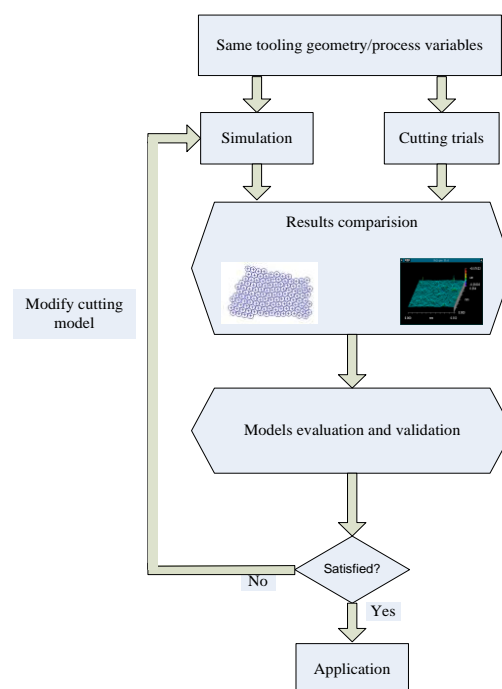


Fig. 11 The procedure for evaluation and validation of the QC model

## 6. Conclusions

In this paper, the QC-based multiscale simulations are presented to investigate the nanometric cutting of single crystal aluminium. The development of a MATLAB-based simulation system is described for easing and simplifying the multiscale modelling and simulation steps. From the simulation results and preliminary experiment trials, the following conclusions can be drawn:

- (1) QC method characterized by the combined MD-FE technique can be effectively applied to the simulation of nanometric cutting to overcome the limitation of MD simulation.
- (2) The mean cutting force during the machining process and internal stress in workpiece material decrease when the rake angle increases.

Currently, the authors are undertaking well-design nanometric cutting trials so as to further evaluate and validate the FE-MD multiscale modelling and simulations. The simulations are also planned to run on a computing grid cluster available in the department in order to get the higher computer power and efficiency. All of those work above will be reported in the near future.

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